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ORTHONORMAL POLYNOMIAL PROJECTION QUANTIZATION: AN ALGEBRAIC EIGENENERGY BOUNDING METHOD

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Abstract. The ability to generate tight eigenenergy bounds for low dimension bosonic or ferminonic, hermitian or non-hermitian, Schrödinger operator problems is an important objective in the computation of quantum systems. Very few methods can simultaneously generate lower and upper bounds. One of these is the Eigenvalue Moment Method (EMM) originally introduced by Handy and Besssis, exploiting the use of semidefinite programming/nonlinear-convex optimization (SDP) techniques as applied to the positivity properties of the multidimensional bosonic ground state for a large class of important physical systems (i.e. those admitting a moments' representation). A recent breakthrough has been achieved through another, simpler, moment representation based quantization formalism, the *Orthonormal Polynomial Projection Quantization Bounding Method* (OPPQ-BM). It is purely algebraic and does not require any SDP analysis. We discuss its essential structure in the context of several one dimensional examples.

Keywords: Eigenvalue bounding methods, hermitian and non-hermitian linear operators.

1. Introduction

The eigenvalue bounding problem for linear ordinary differential equations, or linear partial differential equations (i.e. LODE/LPDE) has been an active area of research for many decades. In the context of quantum physical systems, as represented by the multidimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\overrightarrow{r})+V(\overrightarrow{r})\Psi(\overrightarrow{r})=E\Psi(\overrightarrow{r}), \qquad (1)$$

the generation of upper bounds to the individual discrete state energies is readily obtainable through such well known methods as that of Rayleigh-Ritz (RR) [1]. The challenge has been to find an equally effective lower bound method. A well known lower bound method is that associated with Temple [2]; however, its convergence rate is slow. Nevertheless, it has served as a spring board for other more effective lower bound formulations. Among these is the work by Marmorino et al. [3], and more recently, that of Martinazzo and Pollak [4]. The latter are able to improve upon the convergence rate of Temple's lower bound formulation.

Despite these successes, two important facts remain. The first is that all the above bounding methods require the use of two different bounding formulations. One for the upper bounds (RR), another for the lower bounds. That is, they do not define a unified theoretical framework for simultaneously generating lower and upper bounds. Additionally, these methods are based on a Hilbert space representation for quantum systems, dependent on the existence of hermitian hamiltonians. They are of little relevance for bounding the real/complex eigenenergies of non-hermitian systems, particularly those corresponding to PT-symmetry breaking systems [5–8].

In this work we present a novel approach that can generate tight bounds for the discrete states of bosonic or fermionic, low dimension, systems, regardless if they are hermitian or not. It is referred to as the Orthonormal Polynomial Projection Quantization Bounding Method (OPPQ-BM), as developed by Handy [9]; and based, in part, on a related method, the OPPQ-Approximation Method by Handy and Vrinceanu [10, 11]. Its general structure is outlined in the following sections, through representative one dimensional systems, both hermitian and non-hermitian. We outline the full OPPQ-BM theory within the context of the one dimensional, double well, sextic anharmonic oscillator; and then demonstrate the existence of the key structures necessary for its implementation to the PT symmetry breaking problem with potential $V(x)=ix^3+iax$.

Beyond the theoretical interest in bounds, they are also of practical importance for delicate systems where conventional computational methods may yield widely varying results. That is, the availability of tight bounds allows one to discriminate between competing theories.

One famous problem of this type corresponds to the Quadratic Zeeman (QZM) effect for superstrong magnetic fields. This problem was analyzed through many different types of computational methods, resulting in a wide range of values for the most challenging state to compute: the ground state binding energy. This was reviewed by Le Guillou and Zinn-Justin (LG-ZJ) in the context of their order dependent conformal transformation analysis [12]. Using novel, Moment Problem [13] related, computational methods, Handy, Bessis, et al. [14, 15]. were able to confirm the accuracy of the LG-ZJ analysis, by computing sufficiently

tight bounds to the ground state binding energy. Subsequent studies by Kravchenko et al. [16], and the more recent work by Schimerczek and Wunner [17], developed a different formulation that yielded vastly improved estimates (not bounds). The work by Handy extended OPPQ-BM to the QZM problem, yielding bounds that significantly improved upon, or were competitive with, the estimates by Kravchenko et al.

The QZM problem is an example of an important class of problems for which bounding methods are highly relevant. These are classified as *singular perturbation – strongly coupled* systems. Such systems involve quantum particles subjected to very strong forces, over relatively short length scales. This is inherently a multiscale problem, in keeping with the objectives of wavelet analysis [18, 19], etc.

Our original immersion into the eigenenergy bounding problem was through the study of strong coupling-singular perturbation type systems, such as QZM. The natural framework for regulating these systems is through the use of a non-local, extensive, representation. The power moments provide such a representation. As such, the types of systems studied here are those for which the Schrödinger operator configuration space problem can be transformed into a moments' equation counterpart for the power moments of the bound state solutions. We refer to these as MER type systems (i.e. those admitting a moment equation representation). This will become clear below. This condition can be relaxed, and essentially imposed on systems that do not admit such MER formulations, making the underlying OPPQ-BM principles applicable to many different types of systems. The details of this expanded analysis will be communicated shortly.

1.1. Singular-perturbation strong coupling problems and moment representations

It is not widely appreciated that power moments are relevant in understanding the multiscale structure of most systems. Thus, consider the scaling transform of a given wavefunction (i.e. signal, where we have simplified the notation to that of one dimension):

$$S\Psi(a,b) \equiv \frac{1}{a\nu}\int_{-\infty}^{+\infty} dx\ \mathcal{S}(\frac{x-b}{a})\Psi(x), \qquad (2)$$

where

$$Lim_{a\to 0^+} S\Psi(a,b) = \Psi(b), \qquad (3)$$

and $\nu \equiv \int dx\ \mathcal{S}(x) \neq 0$.

Physicists are biased in favor of attaining an analytical understanding of problems. Therefore the natural question to ask is, what is the analytical dependence in the inverse scale (i.e. $\frac{1}{a}$) for this scaling transform, if Ψ is a bounded, L^2 state? It will become clear from Eq. (4), that the power moments of the bound state solution, determine the analytic structure of the inverse scale expansion. These considerations underlie the analysis by Handy [20].

Alternatively, engineers are more oriented towards computational capabilities. If so, then it readily follows that the $a \to 0$ limit can be replaced by the integral $\int_0^\infty d\alpha \partial_\alpha \Big(\alpha \mathcal{S}\big(\alpha(x-b)\big)\Big)$, where $\alpha \equiv \frac{1}{a}$, which after a convolution substitution gives one the Continuous Wavelet Transform [19].

For bound state configurations, if $\lim_{|x|\to\infty} \Psi(|x|)\mathcal{S}(|x|e^{i\theta}) = 0$, exponentially, for arbitrary θ, then the scaling transform becomes analytic in the inverse scale, $\frac{1}{a}$. Under this assumption, the scaling transform's analytic expansion depends on the moments [20]

$$S\Psi(a,b) = \frac{1}{a\nu}\sum_{j=0}^{\infty}\frac{\sigma_j}{j!a^j}\sum_{p=0}^{j}\binom{j}{p}(-b)^{j-p}\mu(p), \qquad (4)$$

where $\partial_x^j \mathcal{S}(0) \equiv \sigma_j$, and

$$\mu(p) \equiv \int_{-\infty}^{+\infty} dx\ x^p \Psi(x). \qquad (5)$$

2. The moment equation representation

The natural extension of the above considerations is to study linear quantum systems whose differential form is transformable into a moment equation. Thus consider the sextic anharmonic oscillator potential, where the physical parameters have been re-scaled:

$$-\epsilon^2\partial_x^2\Psi(x) + (mx^2 + gx^6)\Psi(x) = E\Psi(x). \qquad (6)$$

The nature of physical quantum systems is that the discrete states decay exponentially, and therefore have finite power moments. The unphysical solutions become exponentially unbounded in one or both asymptotic directions, therefore their power moments are infinite.

We can multiply the above equation by x^p and integrate by parts, assuming the underlying wavefunction is that of a discrete state. We then obtain the *moment equation representation* (MER):

$$\begin{aligned} g\mu(p+6) =& -m\mu(p+2) + E\mu(p) \\ &+ p(p-1)\epsilon^2\mu(p-2), \qquad p \geq 0. \end{aligned} \qquad (7)$$

This homogeneous MER expression is a finite difference equation of effective order $1+m_s$ where $m_s = 5$. That is, for any E parameter value, the first six power moments $\{\mu_0, \mu_1, \ldots, \mu_5\}$ (i.e. $\mu(\ell) \equiv \mu_\ell$) are the initialization moments, or *missing moments*, and generate all the other power moments through closed form, energy dependent coefficients:

$$\mu(p) = \sum_{\ell=0}^{m_s} M_E(p,\ell)\ \mu_\ell, \qquad p \geq 0. \qquad (8)$$

If the coupling strength is large, $g >> 1$, the natural inclination is to attempt some kind of singular perturbation analysis involving expansions around the kinetic energy term; or, alternatively, a large perturbative expansion/resummation analysis.

In configurations space, kinetic energy expansions become singular (i.e. expanding in ϵ^2) because the order of the differential equation abruptly changes from zero to two. However, the order of the MER relation does not change as its kinetic energy counterpart is set to zero. This is one simple evidence that the MER transformation regulates singular perturbation expansions (i.e. kinetic energy expansions). That is, singular perturbation expansions in the moments' representation are better behaved.

3. Generating eigenenergy bounds within a moments' representation

There are two methods for generating bounds within a moment equation representation (MER). The first method, referred to as the Eigenvalue Moment Method (EMM), was developed by Handy and Bessis [14, 15], and is based on the Moment Problem [13]. Its theoretical-computational structure is based on what is now referred to as semidefnite programming (SDP) [21, 22]. As such, the SDP based formulation of Handy and Bessis is the first use of such methods for quantum operators [22]. Its computational implementation was done through the use of linear programming [23], since SDP algorithms were not known in the 1980s.

The second moment representation bounding formulation is that presented in this work, OPPQ-BM. Unlike EMM, OPPQ-BM is applicable to the low lying discrete states of any system, hermitian, or non-hermitian, bosonic, or fermionic, provided it admits a moment equation representation (MER). EMM is applicable only for the multidimensional bosonic ground state.

For systems admitting both EMM and OPPQ-BM, it is our belief that at its basic level, EMM produces faster converging bounds (as shown in this work through the analysis of the sextic anharmonic oscillator in Eq. (6)); however, if one optimizes the selection of the *reference/weight* function, then OPPQ-BM can yield significantly faster converging results.

The EMM formulation involves sophisticated, nonlinear, convex optimization analytical tools. However, OPPQ-BM is purely algebraic (i.e. eigenvalues, eigenvectors, and algebra). Given the power of Mathematica, with unlimited precision, it can produce spectacular results.

It is important to stress that EMM produces (when applicable) tight bounds ab initio. The OPPQ-BM is empirical. If the convergence of a particular parameter is numerically observed, then one can confidently generate bounds for the physical energies. We demonstrate this.

4. The eigenvalue moment method

The bosonic ground state must be a positive (nonnegative) configuration [24], $\Psi_{gr}(\overrightarrow{r}) \geq 0$. If the corresponding Schrödinger equation is transformable into MER form, then one can impose the Moment Problem positivity theorems and constrain the power moments, and in turn the energy and missing moments. This is the EMM-methodology. This was done, several decades ago, by Handy and Bessis (HB) [14, 15].

The Eigenvalue Moment Method (EMM), achieves geometric convergence rates for the bounds to the ground state energy. The only limitation is that it can only be applied to multidimensional bosonic systems, and then only to the ground state. As previously noted, it was used to solve the Quadratic Zeeman (QZM) problem [15]. The bounding of bosonic excited states, through a moment representation, could only be realized more recently through application of OPPQ-BM [9].

One can extend the EMM quantization philosophy to the probability density of one dimensional hermitian Schrödinger operators. This is because the probability density will satisfy a third order, linear, differential equation (LODE). If the LODE representation admits a MER formulation, then one can generate tight bounds to any discrete state. This is because all the discrete states are associated with nonnegative, L^2, configurations.

If the underlying Sturm-Liouville problem is non-hermitian, then the one dimensional Schrödinger equation can be transformed into a fourth order LODE for the probability density. This approach was used by Handy [8] in precisely computing the a-parameter regimes where the system $V(x) = ix^3 + iax$, violated PT symmetry (i.e. PT symmetry breaking). These results were confirmed through a faster, moment based, estimation procedure [25], that led to a more detailed understanding for the onset of PT symmetry breaking. These results significantly improved upon the predictions by Delabaere and Trinh [26], based on asymptotic analysis. We revisit this problem in this work.

The multidimensional probability density, $S(\overrightarrow{r}) \equiv \Psi^*(\overrightarrow{r})\Psi(\overrightarrow{r})$ will not generally satisfy a linear partial differential equation; therefore, no MER relation can be generated, and EMM cannot be applied. Nevertheless, through OPPQ-BM we can circumvent this difficulty.

5. THE ORTHONORMAL POLYNOMIAL PROJECTION QUANTIZATION FORMALISM

5.1. THE OPPQ NON-ORTHOGONAL BASIS EXPANSION

Let us expand the discrete state wavefunction in terms of some appropriate, complete, non-orthonormal basis, $\{\mathcal{B}_n(x) \equiv P_n(x)R(x)\}$:

$$\Psi(x) = \sum_{n=0}^{\infty} c_n P_n(x) R(x). \tag{9}$$

We require a weighted polynomial basis, involving orthonormal polynomials relative to some appropriate positive weight $R(x) > 0$ (we adopt the one dimensional notation for simplicity):

$$\langle P_m | R | P_n \rangle = \delta_{m,n}. \tag{10}$$

The weight is real, as are its orthonormal polynomials, involving real polynomial coefficients:

$$P_n(x) = \sum_{j=0}^{n} \Xi_j^{(n)} x^j. \tag{11}$$

For non-hermitian systems with complex bound state wavefunctions, it is the projection coefficients, $\{c_n\}$ that become complex.

The basis $\{\mathcal{B}_n(x)R(x)\}$ will be complete, but non-orthogonal (i.e. $\langle \mathcal{B}_m | \mathcal{B}_n \rangle \neq 0$, if $m \neq n$).

We can rewrite Eq. (10) as

$$\sum_{j_1=0}^{m} \sum_{j_2=0}^{n} \Xi_{j_1}^{(m)} \omega(j_1 + j_2) \Xi_{j_2}^{(n)} = \delta_{m,n}, \tag{12}$$

where $\omega(j_1 + j_2) = \int dx\ x^{j_1+j_2} R(x)$, the Hankel moment matrix of the weight, $W_{i,j} \equiv \omega(i+j)$.

Knowledge of the Hankel moment matrix allows us to generate the orthonormal polynomials through the Cholesky decomposition method, which involves decomposing the positive Hankel matrix into the form $W = CC^\dagger$. Let $\hat{e}_j$ correspond to a unit vector in the j-th component. We then solve for

$$\overrightarrow{\Xi}^{(j)} = (C^\dagger)^{-1} \hat{e}_j. \tag{13}$$

This generates the coefficient vector for $P_n(x)$, or $\overrightarrow{\Xi^{(n)}}$.

The projection coefficients are obtainable from the MER relation for the power moments of $\Psi(x)$:

$$\mu(p) \equiv \int_{\Re} dx\ x^p \Psi(x). \tag{14}$$

Assume that the corresponding MER relation exists

$$\mu(p) = \sum_{\ell=0}^{m_s} M_E(p,\ell) \mu_\ell. \tag{15}$$

It then follows that

$$\begin{aligned} c_n &= \langle P_n | \Psi \rangle, \\ &= \sum_{j=0}^{n} \Xi_j^{(n)} \mu(j) \\ &= \sum_{j=0}^{n} \Xi_j^{(n)} \sum_{\ell=0}^{m_s} M_E(j,\ell) \mu_\ell, \end{aligned} \tag{16}$$

$$c_n(\overrightarrow{\mu}) = \sum_{\ell=0}^{m_s} \Lambda_\ell^{(n)}(E) \mu_\ell, \tag{17}$$

where

$$\Lambda_\ell^{(n)}(E) = \sum_{j=0}^{n} \Xi_j^{(n)} M_E(j,\ell). \tag{18}$$

The MER relation suggested in Eq. (15) is a homogeneous relation for the power moments. Some normalization condition needs to be imposed:

$$\mathcal{C}(\overrightarrow{\mu}) = 1. \tag{19}$$

For one dimensional systems, the natural normalization is the unit (nonlinear) normalization: $|\overrightarrow{\mu}|^2 = 1$. However, it need not be chosen as such. Alternative choices [9] are linear normalizations such as $\mu_0 = 1$ or $\mu_0 + \mu_1 = 1$, etc.

5.2. THE OPPQ QUANTIZATION CONDITION

The OPPQ quantization condition requires that the weight be chosen so that the following positive integral is bounded for discrete solutions and infinite for unphysical solutions:

$$\mathcal{I}[\Psi, R] = \int_{\Re} dx\ \frac{|\Psi(x)|^2}{R(x)}, \tag{20}$$

$$= \sum_{j=0}^{\infty} |c_j(E, \overrightarrow{\mu})|^2, \tag{21}$$

where we have assumed Ψ is a bounded discrete state.

More generally, we note that depending on the asymptotic behavior of the physical or unphysical (i.e. unbounded) solutions, and the chosen asymptoic form for the weight, the integral in Eq. (20) will satisfy the quantization condition:

$$\mathcal{I}[\Psi, R] = \begin{cases} finite, \iff E = E_{phys}\ and\ \overrightarrow{\mu} = \overrightarrow{\mu}_{phys} \\ \infty, \iff E \neq E_{phys}\ or\ \overrightarrow{\mu} \neq \overrightarrow{\mu}_{phys}. \end{cases} \tag{22}$$

The OPPQ quantization condition essentially becomes a *shooting method* in the $E \times \overrightarrow{\mu}$, $1 + m_s$, parameter space (after imposing a normalization). This is the essence of the OPPQ-BM *bounding procedure*. The focus of the remaining OPPQ formalism is to reduce this shooting method to a minimization problem in the energy parameter space.

5.2.1. Selection of the OPPQ weight

The above formalism has two significant advantages.

The first is that it tells us that the weight should not be chosen so that it asymptotically vanishes much faster than the asymptotic form of the physical solutions.

Thus, given a physical, discrete state, Ψ, let $C(x)$ satisfy the asymptotic relation:

$$Lim_{|x|\to\infty}\frac{\Psi(x)}{R(x)} = C(x). \tag{23}$$

We then want

$$\int dx|\Psi(x)C(x)| < \infty. \tag{24}$$

In the works by Handy and Vrinceanu [10, 11], which introduce a particular version of the OPPQ formalism (i.e. to be referred to here to as the OPPQ-Approximation Method (OPPQ-AM)), they argued and demonstrated that the fastest convergence to the discrete states is associated with weights that mimic the asymptotic form of the desired discrete state:

$$Lim_{|x|\to\infty}C(x) = const. \tag{25}$$

The constant can be finite (i.e. zero), but not infinite in a manner that violates Eq. (24).

5.2.2. Use of the ground state as a weight

Another advantage of the above formalism is that we can take $R(x) = \Psi_{gr}(x)$ even if we do not know the functional form for the ground state.

As long as one does not require that the discrete state wavefunction be reconstructed (i.e. one is only interested in the eigenenergies) then the only information required for the ground state is that its power moments be known accurately. This then allows us to generate the corresponding orthonormal polynomials, allowing for the generation of rapidly converging bounds to the discrete states. We demonstrate this in this work (i.e. Table 8).

One can determine the power moments of the ground state wavefunction either through EMM or OPPQ-BM. Note that for bosonic systems, this is an excellent use of EMM, since the ground state is usually the only state that can be determined.

Using the ground state as a weight usually yields the fastest convergence.

6. The OPPQ-approximation method (OPPQ-AM)

From Eq. (21) and the OPPQ quantization condition in Eq. (22) it follows that the physical energy and missing moment values must satisfy

$$lim_{\to\infty}c_n(E_{phys}, \overrightarrow{\mu}_{phys}) = 0. \tag{26}$$

Since $c_n(E, \overrightarrow{\mu}) = \overrightarrow{\Lambda}^{(n)}(E)\cdot\overrightarrow{\mu}$, from Eq. (17), the $1+m_s$ linear equations

$$\sum_{\ell_2=0}^{m_s}\Lambda_{\ell_2}^{(N-\ell_1)}(E)\ \mu_{\ell_2} = 0, \tag{27}$$

$0 \le \ell_1 \le m_s$, can be used to approximate the physical energies through the determinantal secular equation

$$Det\Big(\Lambda_{\ell_2}^{(N-\ell_1)}(E)\Big) = 0. \tag{28}$$

This defines the OPPQ-Approximation Method (OPPQ-AM). As indicated earlier, Handy and Vrinceanu [10, 11] noted significant improvement in the convergence rates when the weight, R, mimics the asymptotic form of the desired physical states.

The OPPQ representation is very robust, and no convergence irregularities emerge so long as the weight does not decrease much faster than the asymptotic form of the physical states. Provided this is satisfied, the OPPQ-AM formalism will always converge to the true physical energies; however, the rate of convergence depends on the asymptotic properties of the chosen weight.

Despite these impressive results, there is no guarantee that, for hermitian systems, the energies generated through Eq. (28) will be real. Spurious, small imaginary parts may be produced from Eq. (28), that vanish in the $N \to \infty$ limit.

By way of contrast, the OPPQ-Bounding Method to be described below, will always generate real energies for hermitian systems. In addition, as its name suggests, converging bounds to the discrete state energies can be generated.

We make the last observation more explicit. As will be shown below, OPPQ-BM generates, to each order, an energy dependent function, $\mathcal{L}_N(E)$. The local minima, $\partial_E\mathcal{L}_N(E) = 0$ will approximate the physical energies. These local minima can, essentially, be bounded, through converging lower and upper bounds. We refer to the local minima in $\mathcal{L}_N(E)$ as the *OPPQ-BM estimates*, in order to distinguish them from the OPPQ-AM estimates from Eq. (28) and the OPPQ-BM generated bounds.

7. The OPPQ-bounding method

We outline the structure of OPPQ-BM for one space dimension problems. The major difference between one dimensional and multidimensional MER type systems is that one dimensional problems have a fixed number of missing moments: $m_s < \infty$.

Multidimensional problems involve an infinite hierarchy of missing moment subspaces of increasing dimension. That is, $m_s \to \infty$. We develop the 1-space dimension OPPQ formalism in a manner that extends to multidimensions. How the normalization prescription is chosen, plays an important role in the formalism [9].

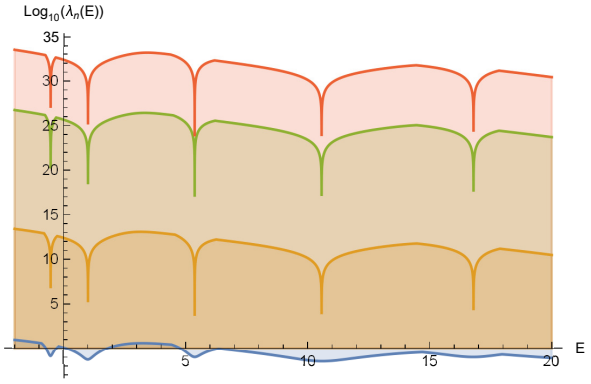

FIGURE 1. $Log_{10}(\lambda_N(E))$ for sextic anharmonic oscillator system in Eq. (47); $N = 20, 40, 100, 120$.

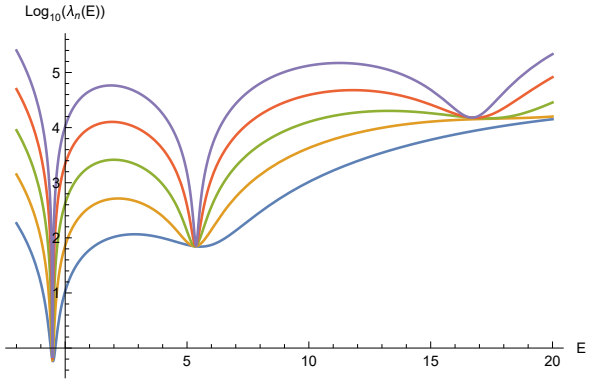

FIGURE 2. $Log_{10}(\lambda_N(E))$ for sextic anharmonic oscillator even states in Eq. (65); $N = 4, 6, 8, 10, 12$; based on the weight $R_L(\xi) = \xi^{-\frac{1}{2}} exp(-\xi)$.

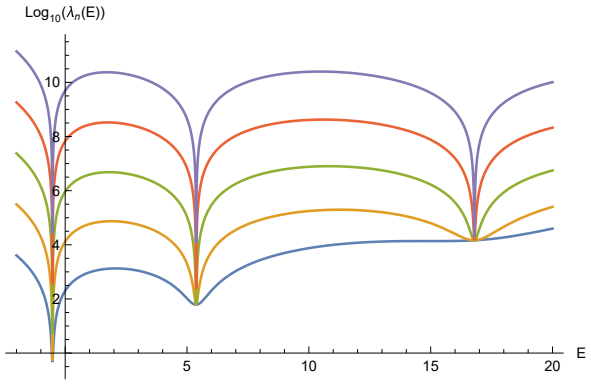

FIGURE 3. $Log_{10}(\lambda_N(E))$ for sextic anharmonic oscillator even states in Eq. (65); $N = 4, 6, 8, 10, 12$; based on the weight $R_G(\xi) = \xi^{-\frac{1}{2}} exp(-\xi^2/2)$.

The OPPQ quantization condition in Eq. (22) is dependent on the positive, (essentially) increasing, sequence, defined by the partial sums:

$$\mathcal{I}[\Psi, R] = Lim_{N\to\infty} S_N(E, \overrightarrow{\mu}), \tag{29}$$

where

$$S_N(E, \overrightarrow{\mu}) = \sum_{j=0}^{N} |c_j(E, \overrightarrow{\mu})|^2, \tag{30}$$

$$= \langle \overrightarrow{\mu} | \mathcal{P}_N(E) | \overrightarrow{\mu} \rangle, \tag{31}$$

where $\mathcal{P}_N(E)$ is an energy dependent, positive matrix (if $N \geq m_s$) of dimension $(1 + m_s) \times (1 + m_s)$:

$$\mathcal{P}_N(E) = \sum_{j=0}^{N} \left(\overrightarrow{\Lambda}^{(j)}(E)\right)^* \overrightarrow{\Lambda}^{(j)}(E), \tag{32}$$

involving the sum over dyad matrix expressions.

For non-hermitian systems, the "*bra*" missing moment vector in Eq. (31) requires the complex conjugate expression for positive norms on complex vector spaces.

It trivially follows, by definition, that

$$0 < S_N(E, \overrightarrow{\mu}) < S_{N+1}(E, \overrightarrow{\mu}) < \ldots < \mathcal{I}[E, \overrightarrow{\mu}]. \tag{33}$$

The OPPQ quantization condition in Eq. (22) tells us that the physical energy and corresponding missing moments correspond to $(E_{phys}, \overrightarrow{\mu}_{phys})$ points within the $E \times \overrightarrow{\mu}$ parameter space where the functional $\mathcal{I}[\Psi, R]$ has a local minimum. Also, for fixed E_{phys}, the corresponding physical missing moment values are those corresponding to a global minimum in the missing moment space. Therefore, to order N we can focus on the global minimum within the constrained (i.e. normalized) missing moment space:

$$\mathcal{L}_N(E) \equiv Inf_{\overrightarrow{\mu}}\{S_N(E, \overrightarrow{\mu}) | \mathcal{C}_{norm}(\overrightarrow{\mu}) = 1\}, \tag{34}$$

where some convenient normalization has been adopted, $\mathcal{C}(\overrightarrow{\mu}) = 1$.

An important result is that

$$\mathcal{L}_N(E) < \mathcal{L}_{N+1}(E). \tag{35}$$

This trivially follows from Eqs. (33-34).

An immediate consequence is that the counterpart to the quantization condition in Eq. (22) now becomes simpler:

$$\lim_{N\to\infty} \mathcal{L}_N(E) = \begin{cases} finite & \Longleftrightarrow \; E = E_{phys}, \\ \infty & \Longleftrightarrow \; E \neq E_{phys}. \end{cases} \tag{36}$$

Combining this with Eq. (35) we obtain:

$$0 < \mathcal{L}_N(E) < \mathcal{L}_{N+1}(E) < \ldots \begin{cases} finite, & \Longleftrightarrow \; E = E_{phys} \\ \infty, & \Longleftrightarrow \; E \neq E_{phys}. \end{cases} \tag{37}$$

Therefore, the $\mathcal{L}_N(E)$ functions form an increasing, nested, concaved upwards, sequence of positive functions. This is demonstrated for the sextic anharmonic harmonic oscillator problem (Figures 1-3), as well as the non-hermitian $ix^3 + iax$ potential (Figure 4), on the complex energy domain. Only at the exact physical energy will the limit be finite. Everywhere else it will become infinite.

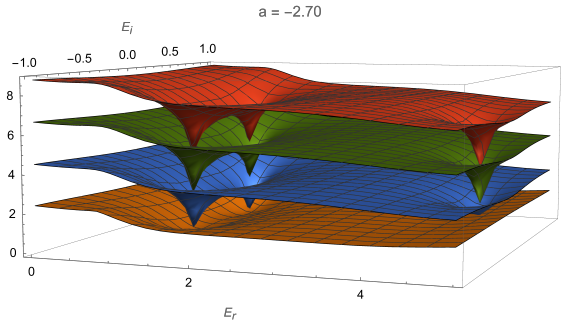

FIGURE 4. $Log_{10}(\lambda_N(E))$ for $N = 20, 30, 40, 50$, $V(x) = ix^3 + iax$, $a = -2.70$

Given the behavior of the $\mathcal{L}_N(E)$, it is clear that the local minima in the energy variable, at a given order "N", should approximate the physical energies. Thus, for each physical discrete state, its corresponding approximants, $E_{phys;N}$, will satisfy

$$\partial_E \mathcal{L}_N(E^{(min)}_{phys;N}) = 0, \tag{38}$$

resulting in

$$\lim_{N\to\infty} E^{(min)}_{phys;N} = E_{phys}. \tag{39}$$

More importantly, these local minima have a very important property. The expressions $\mathcal{L}_N(E^{(min)}_{phys;N})$ form an increasing, positive sequence, bounded from above by the physical counterpart. This follows from

$$\mathcal{L}_N(E^{(min)}_{phys;N}) < \mathcal{L}_{N+1}(E^{(min)}_{phys;N+1}), \tag{40}$$

which follows from:

$$\begin{aligned}\mathcal{L}_N(E^{(min)}_{phys;N}) &< \mathcal{L}_N(E^{(min)}_{phys;N+1}) \\ &< \mathcal{L}_{N+1}(E^{(min)}_{phys;N+1}).\end{aligned} \tag{41}$$

It now follows that the counterpart to the OPPQ quantization condition in Eq. (22) becomes

$$\begin{aligned}0 < \mathcal{L}_N(E^{(min)}_{phys;N}) < \mathcal{L}_{N+1}(E^{(min)}_{phys;N+1}) < \dots \\ < \mathcal{L}_\infty(E_{phys}).\end{aligned} \tag{42}$$

Thus, the $\{\mathcal{L}_N(E^{(min)}_{phys;N})\}$ form a monotonically increasing positive sequence bounded from above by the physical value. The minima do not necessarily converge monotonically.

8. The OPPQ-bounding method

Upon reviewing Eq. (42) a bounding strategy emerges. Assume that the sequence elements can be generated to sufficiently high expansion orders, and that a rough upper bound, $\mathcal{B}_U$ can be discerned:

$$\begin{aligned}\mathcal{L}_N(E^{(min)}_{phys;N}) < \mathcal{L}_{N+1}(E^{(min)}_{phys;N+1}) < \dots \\ < \mathcal{L}_\infty(E_{phys}) < \mathcal{B}_U.\end{aligned} \tag{43}$$

Given the behavior of the $\mathcal{L}_N(E)$ functions, as given in Eqs. (35-37), one can readily determine energy parameter values satisfying

$$\mathcal{L}_N(E^{(L)}_{phys;N}) = \mathcal{L}_N(E^{(U)}_{phys;N}) = \mathcal{B}_U, \tag{44}$$

such that

$$E^{(L)}_{phys;N} < E_{phys} < E^{(U)}_{phys;N}, \tag{45}$$

and

$$\lim_{N\to\infty} \left(E^{(U)}_{phys;N} - E^{(L)}_{phys;N}\right) = 0^+. \tag{46}$$

As a point of comparison, the Rayleigh-Ritz (RR) method solely produces upper bounds. Regardless of how rapidly these bounds converge from above (to the physical value), there is no theoretical criteria by which the RR results can suggest a lower bound to the physical energy. The OPPQ-BM method does.

9. The sextic anharmonic double well potential

The sextic anharmonic oscillator (double well) potential problem is defined by

$$-\partial_x^2\Psi(x) + (x^6 + mx^2)\Psi(x) = E\Psi(x), \tag{47}$$

where we will take $g \equiv 1$ and $m = -4$.

There are three different configuration space representations for the sextic anharmonic oscillator problem, each with different MER relations of varying order. The most immediate is simply working with Ψ as given in Eq. (47). This leads to a sixth order (i.e. $1 + m_s = 6$) finite difference MER relation, as given in Eq. (48). We examine both OPPQ-AM and OPPQ-BM as applied to this representation.

The next configuration space representation is that of the $\Psi^2(x)$ presentation. It leads to a MER relation of order 3 (i.e. $1 + m_s = 3$). We do not apply either OPPQ formulation to this case. However, one can use EMM to bound all the low lying discrete states; thereby providing a test for the effectiveness of OPPQ.

The third, and last, sextic configuration space representation is provided by the contact transformation, $\Phi(x) = exp(-\frac{x^4}{4})\Psi(x)$. This leads to the most efficient MER representation, corresponding to a first order (homogeneous) MER relation (i.e, $1 + m_s = 1$). It results in the fastest OPPQ and EMM convergence.

9.1. EMM-Ψ

The first MER representation to be considered, for the sextic anharmonic oscillator, results from a direct MER analysis of the Schrödinger equation representation in Eq. (47). The power moments along the entire real axis are referred to as the Hamburger moments $\mu(p) = \int_{\Re} dx\ x^p\Psi(x)$.

Upon multiplying both sides of Eq. (47) by x^p and implementing an integration by parts analysis, implicitly assuming that one is working with a discrete state,

there ensues a Hamburger moment equation relation (MER) of the form:

$$\mu(p+6) = -\ m\ \mu(p+2) + E\mu(p) + \ p(p-1)\mu(p-2), \qquad p \geq 0. \quad (48)$$

This is a MER equation of order $1 + m_s = 6$. The MER relation in Eq. (48) applies to both even and odd discrete states.

The generator form for the above MER becomes

$$M_E(p+6,\ell) = -\ m\ M_E(p+2,\ell) + EM_E(p,\ell) + \ p(p-1)M_E(p-2,\ell), \quad (49)$$

$p \geq 0$; and $0 \leq \ell \leq m_s = 5$. The initialization conditions becomes

$$M(\ell_1, \ell_2) = \delta_{\ell_1,\ell_2}, \quad (50)$$

for $0 \leq \ell_{1,2} \leq 5$.

The OPPQ representation becomes

$$\Psi(x) = \sum_{n=0}^{\infty} c_n P_n(x) R(x). \quad (51)$$

One can take the weight to be the Gaussian, $R_G(x) = exp(-x^2)$, or the asymptotic form for the physical states, $R_A(x) = exp(-\frac{x^4}{4})$. In the original formulation of the OPPQ-Approximation Method (OPPQ-AM) Handy and Vrinceanu examined both; and demonstrated the superiority of $R_A(x)$. Our interest here is to demonstrate this approach, and to implement the OPPQ-Bounding Method with regards to the R_A formulation.

The orthonormal polynomials for the Gaussian, $R_G(x)$, are determined by the Hermite polynomials

$$\langle \hat{H}_m | exp(-x^2) | \hat{H}_n \rangle = \delta_{m,n}, \quad (52)$$

or

$$\hat{H}_n(x) = \frac{1}{\sqrt{\sqrt{\pi} 2^n n!}} H_n(x). \quad (53)$$

The orthonormal polynomials (i.e. their coefficients) for $R_A(x)$ are determined through the Cholesky decomposition of the Hankel moment matrix

$$W_{m,n} \equiv \int_{\Re} dx\ x^{m+n} exp(-x^4/4), \quad (54)$$

or

$$W_{m,n} = \begin{cases} 0, \text{if } m+n = odd, \\ 2^{\eta - \frac{1}{2}} \Gamma(\frac{\eta + 1/2}{2}), \text{if } m+n = 2\eta, (\text{even}). \end{cases} \quad (55)$$

The projection coefficients are determined by

$$c_n(E, \mu_0, \ldots, \mu_5) = \sum_{\ell=0}^{m_s=5} \Lambda_\ell^{(n)}(E)\ \mu_\ell, \quad (56)$$

from Eq. (17-18), where

$$\Lambda_\ell^{(n)}(E) = \sum_{j=0}^{n} \Xi_j^{(n)} M_E(j,\ell). \quad (57)$$

The OPPQ-Approximation Method corresponds to solving the secular equation

$$c_{N-\ell_1}(E, \overrightarrow{\mu}) = 0, \quad (58)$$

for $0 \leq \ell \leq 5$ and $N \to \infty$, or

$$Det\Big(\Lambda_{\ell_2}^{(N-\ell_1)}(E)\Big) = 0, \quad (59)$$

a 6×6 determinantal secular equation.

In summary, having chosen N, we need to generate $\{\Lambda_\ell^{(n)}(E) | N - m_s \leq n \leq N\}$. This requires the orthonormal polynomials to order N and the generation of $M_E(p+6,\ell)$, for $0 \leq p \leq N-6$. The Hankel moment matrix for the weight are required up to order $2N$.

The results for both choices of weight are indicated in Tables 1 and 2, for the first ten discrete state energies. It is clear that the R_A choice for the weight is orders of magnitude faster than the simple Gaussian.

It is natural to normalize the missing moments according to a unit normalization $|\overrightarrow{\mu}|^2 = 1$, or

$$\sum_{\ell=0}^{5} \mu_\ell^2 = 1. \quad (60)$$

Accordingly, the energy functional whose minimization is part of the OPPQ-Bounding Method becomes:

$$\mathcal{L}_N(E) \to \lambda_N(E) \equiv \textit{Smallest Eigenvalue of } \mathcal{P}_N(E), \quad (61)$$

where the dyad matrix is given by

$$\Big(\mathcal{P}_N(E)\Big)_{\ell_1,\ell_2} = \sum_{j=0}^{N} \Lambda_{\ell_1}^{(j)}(E) \Lambda_{\ell_2}^{(j)}(E). \quad (62)$$

The $\lambda_N(E)$ form a family of nested, increasing functions, whose local minima approximate the eigenenergies, and serve to define a bounding formalism. We depict this behavior for the $R_A(x)$ weight, in Figure 1. The resolution is not too high and so it is difficult to appreciate that the downward spikes actually are very close to each other. This type of illustration becomes easier to recognize in a subsequent reformulation of the sextic anharmonic oscillator.

We can also apply EMM analysis to the system in Eq. (47). The EMM procedure essentially imposes the well known Hankel Hadamard Moment Problem constraints in order to bound the discrete state energies associated with nonnegative configuration space solutions. Since the only state of this type is the ground state, which must also be of even parity, we can further specialize the MER relation in Eq. (48) to

N	E_0	E_1	E_2	E_3	E_4
25	-0.530376450630854	0.985067365669966	5.28830977093027	10.4934190522107	15.8338485774860
50	-0.523284216533135	1.00560182885171	5.37480811122565	10.5699924952422	16.7909114406834
75	-0.523268805558542	1.00576819439460	5.37496683348150	10.5725844031665	16.7952741272760
100	-0.523268623704744	1.00576834791848	5.37496999430605	10.5725850991710	16.7953468181267
125	-0.523268622109697	1.00576834035184	5.37497000920767	10.5725850451529	16.7953468448794
150	-0.523268622126032	1.00576834023041	5.37497000886154	10.5725850446303	16.7953468331754
175	-0.523268622127498	1.00576834022567	5.37497000884083	10.5725850445874	16.7953468327220
200	-0.523268622127550	1.00576834022555	5.37497000884007	10.5725850445860	16.7953468327042
25	-0.523268576015852	1.00576828117312	5.37497437050670	10.5726072299740	16.7951977796668
50	-0.523268622127552	1.00576834022554	5.37497000884005	10.5725850445859	16.7953468327034
100	-0.523268622127552	1.00576834022554	5.37497000884004	10.5725850445859	16.7953468327036
200.	-0.523268622127552	1.00576834022554	5.37497000884004	10.5725850445859	16.7953468327036

TABLE 1. OPPQ-AM, for the first five states of $V(x) = x^6 - 4x^2$, $m_s = 5$, $R_{Gauss} = e^{-x^2}$ and $R_A = e^{-x^4/4}$.

N	E_5	E_6	E_7	E_8	E_9
25	23.5770262257055	46.5131514442214			
50	23.8599097864908	31.6506317849753	40.1684238879451	48.7083019153321	57.2184300245252
75	23.8838452220218	31.7416917119713	40.2993336329482	49.5062748750452	59.2851256940478
100	23.8839209143498	31.7425529172254	40.3026888622591	49.5114653542220	59.3258556535193
125	23.8839223617171	31.7425500612024	40.3027376770457	49.5115009782085	59.3262796515870
150	23.8839223760489	31.7425498440774	40.3027378004240	49.5115004143879	59.3262744628777
175	23.8839223758291	31.7425498374411	40.3027377924283	49.5115003807374	59.3262741019580
200	23.8839223758112	31.7425498371238	40.3027377918922	49.5115003775253	59.3262740863702
25	23.8828743775059	31.7384980035506	40.3209134822543	50.0634788389675	
50	23.8839223758082	31.7425498371192	40.3027377921622	49.5115003777545	59.3262740709658
100	23.8839223758101	31.7425498371122	40.3027377918721	49.5115003773799	59.3262740857373
150	23.8839223758101	31.7425498371122	40.3027377918721	49.5115003773799	59.3262740857373
200	23.8839223758101	31.7425498371122	40.3027377918721	49.5115003773799	59.3262740857373

TABLE 2. OPPQ-AM, for the sixth-tenth states of $V(x) = x^6 - 4x^2$, $m_s = 5$, $R_{Gauss} = e^{-x^2}$ and $R_A = e^{-x^4/4}$.

such states, yielding a reduced finite order difference equation for the power moments (i.e. $m_s = 2$). The results produced bounds to the 8th decimal place for the ground state energy. We obtain the EMM bounds: $-0.523268623844284 < E_{gr} < -0.523268619253327$, based on an expansion order of approximately 29 power moments (i.e. $\{\mu(p)|0 \leq p \leq 28\}$). This was done on a simple PC with about 14 place precision.

We note that the EMM bounds quoted above were accurate to approximately eight decimal places, based on approximately 28-29 power moments. The missing moment order used for the even state formulation was $m_s = 2$. The OPPQ-BM bounds quoted in Table 3, based on an $m_s = 5$ MER formulation, use an optimal weight, but only give us two decimal place accuracy on the basis of 25 power moments. Of course, the bounds quickly improve, as $N \to 125$. We continue these EMM versus OPPQ comparisons below.

By way of contrast, the OPPQ-BM procedure can produce bounds on all the low-lying states. To produce these, we must first generate the local minima, $\partial_E \lambda_N(E^{(min)}_{phys;N}) = 0$. Fortunately, these derivatives can be obtained algebraically through a recursion procedure. Following this, we must discern a crude upper bound (i.e. $\mathcal{B}^{(U)}_{phys}$) to the positive sequence $\{\lambda_N(E^{(min)}_{phys;N})|N > 0\} < \mathcal{B}^{(U)}_{phys}$. We then determine the energy interval whose endpoints satisfy $\lambda_N(E^{(L)}_{phys;N}) = \mathcal{B}^{(U)}_{phys} = \lambda_N(E^{(U)}_{phys;N})$. These become the lower and upper bound estimates for that physical energy.

The above bounding analysis is initiated in Table 4 for the ground and second excited state of the sextic anharmonic oscillator. Since the use of the R_A weight yields very rapid convergence, we see that the coarse upper bounds, $\mathcal{B}^{(U)}$ are easily determined. Using these we can generate the bounds for the ground state and first excited state, as given in Table 3. We note that the OPPQ-BM bounds generated in Table 3 (we could have continued tightening the bounds), for the ground state, used 125 power moments giving us bounds at the 18th decimal place. In Eq. (69) we quote the EMM bounds obtained on the basis of 61 power moments. The accuracy is at the 33rd decimal place. However, in Eq. (70), using an optimal (Stieljes representation) weight, the OPPQ-AM converged to 50 decimal places, using only 45 power moments.

N	$E^{(L)}_{0;N}$	$E^{(U)}_{0;N}$	$E^{(L)}_{2;N}$	$E^{(U)}_{2;N}$
25	-0.524852943468474	-0.521778245307431	5.368449680815753	5.384374689469648
50	-0.523268749143883	-0.523268495112775	5.374969291406036	5.374970726288986
75	-0.523268622134517	-0.523268622120587	5.374970008804361	5.374970008875728
100	-0.523268622127553	-0.523268622127552	5.3749700088400432	5.3749700088400468
125	-0.52326862212755223948	-0.52326862212755223934	5.3749700088400449937	5.3749700088400449945
		$\mathcal{B}^{(U)} = -0.876$		$\mathcal{B}^{(U)} = -0.990$

TABLE 3. OPPQ-BM upper and lower bounds for the ground and second excited states, using $R_A = e^{-x^4/4}$.

N	$\partial_E \lambda(E^{(min)}_{0;N}) = 0$	$Log_{10}\Big(\lambda(E^{(min)}_{0;N})\Big)$	$\partial_E \lambda(E^{(min)}_{2;N}) = 0$	$Log_{10}\Big(\lambda(E^{(min)}_{2;N})\Big)$
25	-0.523315367444853	-0.877054685910968	5.37640170043752	-0.991603081677466
50	-0.523268622128326	-0.877042389134943	5.37497000884746	-0.991530473233468
75	-0.523268622127552	-0.877042389134815	5.37497000884004	-0.991530473233135
100	-0.523268622127552	-0.877042389134815	5.37497000884004	-0.991530473233135
		$\mathcal{B}^{(U)} = -0.876$		$\mathcal{B}^{(U)} = -0.990$

TABLE 4. OPPQ-BM Analysis for determining coarse upper bounds, $\mathcal{B}^{(U)}$, for the ground and second excited states, using $R_A = e^{-x^4/4}$.

9.2. EMM-Ψ^2

Another MER representation for the sextic anharmonic oscillator is possible by working with the probability density, $S(x) = \Psi^2(x)$. It is easy to show that the probability density for real potentials satisfies a third order LODE. For the sextic anharmonic oscillator problem, this 3rd order LODE yields a MER relation of order 3 (i.e. $m_s = 2$). We do not give the details of this analysis, since the following MER representation offers the easiest OPPQ implementation. The value of EMM-Ψ^2 is that we can bound the discrete states and use the results to gauge the effectiveness of OPPQ. This is referenced below.

9.3. EMM $e^{-\frac{x^4}{4}}\Psi(x)$

The third MER representation is obtained through the contact transformation,

$$\Phi(x) = exp(-\frac{x^4}{4})\Psi(x). \tag{63}$$

Since this involves a factor identical to the dominant WKB asymptotic form for the physical states, the MER representation for Φ will involve fewer missing moments (i.e. none, after a normalization) than the MER for Ψ, as given in Eq. (48), involving five (5) missing moments (after imposing a normalization). This is desirable since the lower the missing moment order, the faster the convergence of either OPPQ or EMM. We provide the details of both approaches below.

9.4. OPPQ ANALYSIS OF THE $(m_s = 0)$ SEXTIC ANHARMONIC DOUBLE WELL OSCILLATOR

The double well anharmonic problem of interest is that for the potential $V(x) = x^6 - 4x^2$, where $x \in \Re$. The physical solutions must die off, asymptotically, according to the dominant WKB expression $\Psi(x) \sim exp(-\frac{x^4}{4})$.

If we work with the contact transformation in Eq. (63) $\Phi(x) = exp(-\frac{x^4}{4})\Psi(x)$, we note that the discrete states remain normalizable and exponentially bounded, in the Φ representation. Unphysical Ψ configurations (i.e. non-normalizable due to their exponentially unbounded form in one or both asymptotic directions) map into non-normalizable Φ configurations. The EMM formalism works in either representation, precisely because of this. We note that the power moments for exponentially bounded configurations exist; whereas they become infinite (or do not exist) for unphysical configurations.

The Φ configurations must satisfy the differential equation

$$\Phi''(x) + 2x^3\Phi'(x) + (7x^2 + E)\Phi(x) = 0. \tag{64}$$

The Hamburger moment (i.e. $\mu(p) \equiv \int_{\Re} dx\ x^p\Phi(x)$) equation becomes

$$(2p-1)\mu(p+2) = p(p-1)\mu(p-2) + E\mu(p).$$

The even parity states will admit a MER for the even order power moments, $\mu(2\rho) = u(\rho)$ or

$$(4\rho-1)u(\rho+1) = 2\rho(2\rho-1)u(\rho-1) + Eu(\rho). \tag{65}$$

The odd parity states $\mu(2\rho+1) \equiv \nu(\rho)$ will satisfy the MER :

$$(4\rho+1)\nu(\rho+1) = 2\rho(2\rho+1)\nu(\rho-1) + E\nu(\rho). \tag{66}$$

We note that the even order Hamburger moments satisfy: $\mu(2\rho) = u(\rho) = \int_0^{+\infty} d\xi\ \xi^{\rho-1/2}\Phi(\sqrt{\xi})$, where $x^2 = \xi$; however, the odd order Hamburger moments satisfy $\mu(2\rho+1) = \nu(\rho) = \int_0^{+\infty} d\xi\ \xi^{\rho}\Phi(\sqrt{\xi})$. The importance of these relations is that the respective

N	E_0	E_2	E_4	E_6	E_8
10	-0.5234534028	5.354166238	16.82887249		
20	-0.5232677208	5.375031586	16.79298386	31.63171200	49.94322409
30	-0.5232686293	5.374969341	16.79536744	31.74329539	49.45632020
40	-0.5232686220	5.374970019	16.79534604	31.74254727	49.51247497
50	-0.5232686221	5.374970009	16.79534686	31.74254902	49.51148774
60	-0.5232686221	5.374970009	16.79534683	31.74254987	49.51149946
70	-0.5232686221	5.374970009	16.79534683	31.74254984	49.51150043
80	-0.5232686221	5.374970009	16.79534683	31.74254984	49.51150038
90	-0.5232686221	5.374970009	16.79534683	31.74254984	49.51150038
100	-0.5232686221	5.374970009	16.79534683	31.74254984	49.51150038

TABLE 5. OPPQ-BM Estimates (i.e. $\partial_E \lambda_N(E^{(min)}_{phys;N}) = 0$), Φ representation, (Eq. 65) $R_L(\xi) = \xi^{-\frac{1}{2}} exp(-\xi)$.

moments, in the context of Eqs. (65, 66) allow us to implement a Stieltjes moment analysis through EMM.

We will only apply OPPQ on the even Ψ configurations, for simplicity. However, since the even order power moments are the moments of $\Upsilon(\xi) \equiv \frac{\Phi(\sqrt{\xi})}{\sqrt{\xi}}$, the OPPQ expansion must be relative to this configuration. Thus, the relevant OPPQ expansion will be

$$\Upsilon(\xi) = \sum_{n=0}^{\infty} c_n P_n(\xi) R(\xi), \tag{67}$$

where Φ's power moments will satisfy Eq. (65).

Since the physical configurations behave, asymptotically, as $\Psi(x) \sim exp(-\frac{x^4}{4})$, the transformed expressions behave as $\Phi(\xi) \sim exp(-\frac{\xi^2}{2})$.

Since the transformed system involves a Stieltjes configuration supported on the nonnegative axis, one might take the weight to be the exponential function, $\tilde{R}_L(\xi) = exp(-\xi)$, with Laguerre polynomials; or the Gaussian $\tilde{R}_G(\xi) = exp(-\xi^2/2)$, restricted to the nonnegative real axis. However, for the quantization integral in Eq. (20) to apply, particularly with regards to the generation of bounds, we need to take into account the $\xi^{-\frac{1}{2}}$ that is inherent to the transformed, even order, power moments.

Based on the previous arguments we will work with $R_L(\xi) = \xi^{-\frac{1}{2}} exp(-\xi)$ and $R_G(\xi) = \xi^{-\frac{1}{2}} exp(-\xi^2/2)$. The corresponding power moments for the weights, in order to generate the orthonormal polynomials are obtained as follows.

The power moments $w_L(p) \equiv \int_0^\infty d\xi\ \xi^p R_L(\xi)$ or $w_L(p) = \Gamma[p + \frac{1}{2}]$ satisfy the recursion relation $w_L(p+1) = (p + 1/2) w_L(p)$; whereas $w_G(p) \equiv \int_0^\infty d\xi\ \xi^p R_G(\xi)$, or $w_G[p] = 2^{\frac{2p-3}{4}} \Gamma[\frac{2p+1}{4}]$, satisfy the recursion relation $w_G(p+2) = (p + 1/2) w_G(p)$.

In their original work on the OPPQ-Approximation Method (i.e. Eq. (28)), Handy and Vrinceanu implemented OPPQ-AM with both of these types of weights (i.e. using their counterparts along the entire real axis, $x \in \Re$). They showed that superior (faster converging) results were obtained for weights that emulated the asymptotic form of the physical states.

The enhanced efficiency of working with $R_G(\xi)$ instead of $R_L(\xi)$ is evident in Figure 3 compared to Figure 2 (i.e. the functions for the former are converging much faster around the physical energies).

The numerical results for the $m_s = 0$ sextic anharmonic oscillator problem are given in the following section. We only give numerical results based on using $R_L(\xi)$. Instead of working with $R_G(\xi)$, we will use the actual ground state wavefunction (i.e. its power moments), $R_{gr}(\xi)$. The reason is that both have the same asymptotic behavior. That is, $R_{gr}(\xi) = \Phi_{gr}(\xi) \sim R_G(\xi)$; therefore, upon solving for the power moments of the ground state wavefunction (including the energy), we can use it to generate its orthonormal polynomials, and quantize the excited states, through OPPQ.

To be able to do this requires sufficient accuracy in the determination of the ground state power moments, since these must generate a positive Hankel matrix for the weight (before implementation of a Cholesky analysis). Although this can be done through OPPQ, EMM inherently works with positive matrices and therefore is more efficient for doing this type of analysis.

9.5. OPPQ RESULTS FOR THE $m_s = 0$, SEXTIC ANHARMONIC OSCILLATOR

The OPPQ-Φ formulation is a zero missing moment problem (i.e. $m_s = 0$) and converges very fast.

In Figure 2 we plot the nested sequence $\lambda_N(E)$, for $N = 4, 6, 8, 10, 12$. This calculation was done based on the $R_L(\xi)$ weight. A similar result holds for the $R_G(\xi)$ weight as depicted in Figure 3. It clearly reveals the faster convergence afforded by a weight that emulates the asymptotic form of the physical states.

In Table 5 we give the OPPQ-BM energy estimates (i.e. the local minima, $\partial_E \lambda_N(E^{(min)}_{phys.;N}) = 0$) for the low lying, even parity, discrete state energies, based on Eq. (65), using the inferior weight $R_L(\xi) = \xi^{-\frac{1}{2}} exp(-\xi)$.

Table 5 only cites results (to ten significant figures) for $N \leq 100$. Not shown in Table 5 are the OPPQ-BM estimation results for the ground state at $N = 120$:

N	$\partial_E S_N(E_N^{(min)}) = 0$	$Log(S_N(E_N^{(min)}))$	$c_N(E_N) = 0$	$E_N^{(L)}$	$E_N^{(U)}$
20	49.94322409213197	7.982552803	49.4426432537	48.893	50.857
30	49.45632020275004	7.997267757	49.4986057623	49.366	49.546
40	49.51247497421839	8.002499541	49.5123070944	49.504	49.520
50	49.51148774312169	8.002657778	49.5114731270	49.510	49.512
60	49.51149945726214	8.002665930	49.5115007312	49.51140	49.51159
70	49.51150043370514	8.002667120	49.5115003992	49.51148	49.51151
80	49.51150037650008	8.002667337	49.511500375879294	49.5114990	49.5115017
90	49.51150037729806	8.002667346	49.511500377394135	49.5115001949	49.5115005597
100	49.51150037738496	8.002667348	49.511500377382972	49.5115003518	49.5115004029
110	49.51150037737999	8.002667348	49.511500377379789	49.5115003736	49.5115003811
120	49.51150037737991	8.002667348	49.511500377379918	49.5115003768	49.5115003780
		$\mathcal{B} = 8.01$			

TABLE 6. OPPQ Results for E_8: $R_L = \frac{e^{-\xi}}{\sqrt{\xi}}$.

$E_{gr} = -.52326862212755224$. This result lies within the bounds generated through an EMM-Φ analysis (based on the first 29 power moments):

$$-.5232686221275616 < E_{gr} < -.5232686221275495. \quad (68)$$

We can infer that the EMM bounds in Eq. (68) predict the exact answer to 13 decimal places. This result, based on 29 moments, surpasses the OPPQ-BM estimation analysis in Table 5 ($N = 30$) of -0.5232712343, at the fourth-fifth decimal place. Thus EMM-Φ, by this comparison, is approximately three times more efficient.

Having said this, we remind the reader that whereas EMM involves sophisticated analysis (i.e. nonlinear convex optimization), OPPQ is purely algebraic, and implementable to arbitrary accuracy through algebraic software, such as Mathematica. Additionally, EMM is, in practice, only applicable to the (multidimensional) bosonic ground state; whereas OPPQ applies to any multidimensional bosonic or fermionic (low dimension) system, including non-hermitian systems.

9.5.1. GENERATING BOUNDS FOR E_8

We re-examine the results in Table 5 for E_8, the slowest converging energy. As with other methods, such as Rayleigh-Ritz (RR), the manifest convergence of the results (i.e. the $N \to 120$ sequence in Table 5) is no guarantee of the accuracy of the apparent limit in predicting the true energy. Whereas EMM produces converging bounds from first principles; OPPQ defines a procedure by which one can generate bounds provided a certain parameter is empirically determined, specifically the *coarse upper bound*, $\mathcal{B}^{(U)}$. Below we describe the OPPQ-BM bounding procedure in detail, although the same underlies the results in Tables 4 and 3, for the $m_s = 3$ MER formulation in Eq. (48). The only advantage of the current problem is that it is a zero missing moment problem, and therefore easier to implement.

In Table 6 we provide the OPPQ-BM eigenenergy estimate for E_8 (the second column). The third column contains the increasing, convergent, positive sequence from which a coarse upper bound, $\mathcal{B}^{(U)}$, is to be empirically determined. Using this coarse upper bound, we can generate arbitrarily tight bounds (i.e. the last two columns), as $N \to \infty$. Note that we continued generating these bounds in Table 7. This entire procedure is based on the assumption that the manifest convergence of the third column in Table 6 is correctly bounded, from above, by the empirically determined coarse upper bound, $\mathcal{B}^{(U)}$. The fourth column contains the OPPQ-AM estimate.

It is important to appreciate that the coarseness of $\mathcal{B}^{(U)}$ has nothing to do with the tightness of the bounds, in principle, assuming one can generate high OPPQ expansion orders.

Below we compare the accuracy of the OPPQ-BM formalism to order $N - 120$, both with respect to the OPPQ-BM energy estimate ($E_8 = 49.5115003774$, from Table 6) and the OPPQ-BM bounds ($49.5115003768 < E_8 < 49.5115003780$, also from Table 6), as compared to the bounds generated by an EMM analysis. The results are very good and consistent.

It is important to note that the OPPQ-BM estimate obtained at lower order, does not have to lie within the OPPQ-BM bounds obtained at higher order. Thus the entry in the second column in Table 6, corresponding to OPPQ-BM energy estimate (i.e. the local minima) of $E = 49.51148774312169$ (i.e. $N = 50$), lies outside of the bounds generated in the last two columns, for $N > 80$. However, all OPPQ-BM estimates must lie within the bounds calculated at lower order.

9.6. COMPARISON WITH EMM BOUNDS

Generally, the EMM analysis will be more efficient in generating bounds than OPPQ-BM. That is, fewer moments will be required to generate the same level of tightness of the bounds. However, this depends

N	$E_8^{(L)}$	$E_8^{(U)}$
150	49.511500377377302482	49.511500377382545933
160	49.511500377379459378	49.511500377380389040
170	49.511500377379839286	49.511500377380009132
180	49.511500377379908253	49.511500377379940166
190	49.511500377379921131	49.511500377379927287
200	49.511500377379923601	49.511500377379924818
210	49.511500377379924086	49.511500377379924333
220	49.511500377379924184	49.511500377379924235
230	49.511500377379924204	49.511500377379924215
240	49.511500377379924208	49.511500377379924210
250	49.51150037737992420904883O	49.51150037737992420955895 3
260	49.51150037737992420924685 1	49.51150037737992420936093 2
270	49.51150037737992420929091 4	49.51150037737992420931686 9
280	49.51150037737992420930089 0	49.51150037737992420930689 3
290	49.51150037737992420930318 6	49.51150037737992420930459 7
300	49.51150037737992420930372 3	49.51150037737992420930406 0
	$\mathcal{B} = 8.01$	

TABLE 7. Bounds for E_8 based on chosen $\mathcal{B}^{(U)}$.

N	E_0	E_2	E_4	E_6	E_8
1	-0.5232686221275529				
5	-0.5232686221276021	5.37847969429	16.78604192264		
10	-0.5232686221275522	5.37497046837	16.79542276464	31.74535880954	49.5248113799
20	-0.5232686221275523	5.37497000884	16.79534683270	31.74254983720	49.5115003841
30	-0.5232686221275523	5.37497000884	16.79534683270	31.74254983711	49.5115003772

TABLE 8. OPPQ-BM Estimates (i.e. $\partial_E S_N(E) = 0$) for $V(x) = x^6 - 4x^2$, $m_s = 0$, $R(x) = \Phi_{gr}(x)$ based on the first 61, EMM generated, ground state power moments $\{u_{gr}(p \leq 60)\}$.

on the choice of weight, as the following case exemplifies. Thus, with regards to the $m_s = 2$ missing moment formulation given earlier, the EMM bounds for the ground state $-0.523268623844284 < E_{gr} < -0.523268619253327$, were based on the first 29 power moments. The same (approximately) level of tightness was achieved with OPPQ-BM using more than 50 power moments, based on the results in Table 3. Thus, in this example EMM is vastly superior to OPPQ-BM. However, for the next example the situation significantly improves for OPPQ-BM over EMM.

For the $m_s = 0$ formulation being considered, using the first 62 Stieljes power moments (i.e. $\{u(p)|p \leq 61\}$), EMM achieves the bounds:

$$-.523268622127552239416169497190784061165647716306044 < E_{EMM} < -.523268622127552239416169497190784061165647716306035 \quad (69)$$

Using the weight R_L the OPPQ-AM estimate achieves this level of accuracy on the basis of approximately 220 power moments; whereas the weight R_G generates an OPPQ-AM estimate that surpasses the EMM accuracy based only on the use of 45 moments (OPPQ-AM):

$$E_{OPPQ-AM} = -0.523268622127552239416169497190784061165647716306044 \quad (70)$$

9.7. USING THE GROUND STATE AS A WEIGHT

In Table 8 we implement OPPQ-BM on a representation that uses the generated moments of the unknown ground state $R(x) = \Psi_{gr}(x)$. As expected, the convergence is very fast in comparison with results based on R_L.

9.8. EMM RESULTS FOR THE PROBABILITY DENSITY

Application of EMM to the probability density (i.e. EMM-Ψ^2, an $m_s = 2$ problem) yields the bounds $-.52326866 < E_0 < -.52326857$, $1.0057681 < E_1 < 1.0057685$, $5.3749699 < E_2 < 5.3749701$, $10.5725845 < E_3 < 10.5725855$, $16.795339 < E_4 < 16.795351$, $23.883886 < E_5 < 23.883961$, $31.74217 < E_6 < 31.74323$, $40.301 < E_7 < 40.305$, $49.506 < E_8 < 49.533$ all to the same moment expansion order of 28. We also note that an EMM-$\Psi\{m_s = 2\}$ bounding formulation on the ground state yields comparable bounds using the first 28 power moments: $-.5232686237 < E_{gr} < -.5232686193$. With regards

to E_8, extension of EMM-$\Psi^2\{m_s=2\}$ analysis to the first 48 moments (i.e. $\{u(p)|0\le p\le 47\}$) yields the bounds $49.5115003768 < E_8 < 49.5115003798$. These serve to further confirm some of the results previously cited.

10. A PT-symmetry breaking, non-hermitian, problem

Consider the non-hermitian system

$$-\partial_x^2\Psi(x)+(ix^3+iax)\Psi(x)=E\Psi(x), \quad (71)$$

which is known to break PT symmetry for negative values of the 'a' parameter ($a<-2.611809356$, and for $a<-5.375879629$) from Refs. [8, 25]. The case $a=0$ has purely real eigen-energies, as computed by Bender and Boettcher [5], and theoretically confirmed by Dorey et al. [6]. The EMM-$\Psi^*\Psi$ formulation also provided strong numerical evidence for this [27].

States that are PT symmetric satisfy $\Psi^*(-x)=\Psi(x)$, and have real energies, $E\in\Re$. States that break this symmetry have complex conjugate pairs for the energies (i.e. $\Psi^*(-x)\neq\Psi(x)$, with complex energies E^* and E, respectively).

We work with the MER-Ψ representation for which the complex power moments on the real axis satisfy

$$\begin{aligned}\mu(p+3)=&-a\mu(p+1)-iE\mu(p)\\&-ip(p-1)\mu(p-2),\qquad p\ge 0.\end{aligned} \quad (72)$$

The recursion relation for the energy dependent generator coefficients is

$$\begin{aligned}M_E(p+3,\ell)=&-aM_E(p+1,\ell)-iEM_E(p,\ell)\\&-ip(p-1)M_E(p-2,\ell),\end{aligned} \quad (73)$$

for $p\ge 0$, $0\le\ell\le 2$, and $M_E(\ell_1,\ell_2)=\delta_{\ell_1,\ell_2}$. This is an $m_s=2$ representation of order 3. Since the asymptotic form of the physical states goes as $\Psi(x)\sim exp(-\frac{2}{5}|x|^{\frac{5}{2}})$, we can use the Gaussian weight $R(x)=exp(-x^2/2)$. The OPPQ-BM formalism ensues as before:

$$\Psi(x)=\sum_{j=0}^{\infty}c_jP_j(x)R(x), \quad (74)$$

involving real weights and corresponding orthonormal polynomials. The complex projection coefficients are given by

$$c_j(E,\mu_0,\mu_1,\mu_2)=\langle P_j(x)|\Psi\rangle, \quad (75)$$

or

$$c_j(E,\mu_0,\mu_1,\mu_2)=\sum_{\ell=0}^{m_s=2}\Lambda_\ell^{(j)}(E)\ \mu_\ell, \quad (76)$$

where the coefficients depend on the orthonormal polynomial coefficients and the $M_E(p,\ell)$'s:

$$\Lambda_\ell^{(j)}(E)=\sum_{\eta=0}^{j}\Xi_\eta^{(j)}M_E(\eta,\ell). \quad (77)$$

The OPPQ-BM quantization condition is

$$\begin{aligned}\mathcal{I}[\Psi,R]&=\int_{\Re}dx\frac{\Psi^*(x)\Psi(x)}{R(x)}\\&=\begin{cases}finite \iff E=E_{phys}\ and\ \overrightarrow{\mu}=\overrightarrow{\mu}_{phys},\\ \infty\iff E\neq E_{phys}\ or\ \overrightarrow{\mu}\neq\overrightarrow{\mu}_{phys}.\end{cases}\end{aligned} \quad (78)$$

We adopt the vector notation for the missing moments $\overrightarrow{\mu}\equiv(\mu_0,\mu_1,\mu_2)$.

Substituting the OPPQ representation we obtain:

$$\mathcal{I}[\Psi,R]=\sum_{j=0}^{\infty}c_j^*(E,\overrightarrow{\mu})c_j(E,\overrightarrow{\mu}). \quad (79)$$

Once again, the focus is on :

$$\begin{aligned}&S_N(E,\overrightarrow{\mu})\\&\quad=\sum_{\ell_1=0}^{m_s}\sum_{\ell_2=0}^{m_s}\mu_{\ell_1}^*\Big(\sum_{j=0}^{N}\Lambda_{\ell_1}^{(j)}(E)^*\Lambda_{\ell_2}^{(j)}(E)\Big)\mu_{\ell_2},\end{aligned} \quad (80)$$

involving the positive definite matrix

$$\big(\mathcal{P}_N(E)\big)_{\ell_1,\ell_2}=\sum_{j=0}^{N}\Lambda_{\ell_1}^{(j)}(E)^*\Lambda_{\ell_2}^{(j)}(E). \quad (81)$$

If we adopt a unit missing moment vector normalization, then the focus for OPPQ-BM quantization is on the behavior of the smallest eigenvalue, $\lambda_N(E)\equiv$ Smallest Eigenvalue$\Big(\mathcal{P}_N(E)\Big)$, viewed as a function of the real and imaginary parts of the energy variable. The focus is on determining the local minima: $\partial_{E_r}\lambda_N(E_{N,phys}^{(min)})=\partial_{E_i}\lambda_N(E_{N,phys}^{(min)})=0$. These derivatives can be obtained algebraically.

We outline the essential steps for algebraically generating the partial derivatives. First of all, we have $\lambda_N(E)=\langle\overrightarrow{\mu}|\mathcal{P}_N(E)|\overrightarrow{\mu}\rangle$, involving the normalized missing moment (lowest) eigenvector. This is not an analytic function in E, so we must work with the partial derivatives with respects to $E_{r,i}$. Thus, we need $\partial_{E_{r,i}}\lambda_N(E)=\langle\overrightarrow{\mu}|\partial_{E_{r,i}}\mathcal{P}_N(E)|\overrightarrow{\mu}\rangle$. We can generate the required matrix expression from Eq. (80) or $\partial_{E_{r,i}}\mathcal{P}_N(E)=\sum_{j=0}^{N}\Big(\partial_{E_{r,i}}\Lambda^{(j)}(E)^*\Big)\Lambda^{(j)}(E)+c.c.$. From Eq. (77), so long as the Ξ's do not depend on the energy parameter, we need $\partial_{E_{r,i}}M_E(\eta,\ell)$. However, this can be obtained recursively through the expression in Eq. (72).

Our immediate interest is on the behavior of $\lambda_N(E)$ over the two dimensional complex energy plane, as the parameter 'a' is varied, and $N=40$. In Figures 5-12 we show the convergence of two PT-breaking (complex conjugate) energies (eventually becoming real) as we increase the a-parameter through

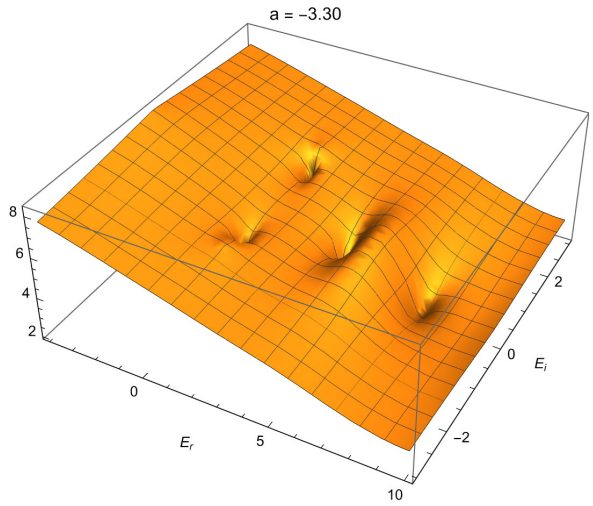

FIGURE 5. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -3.30$

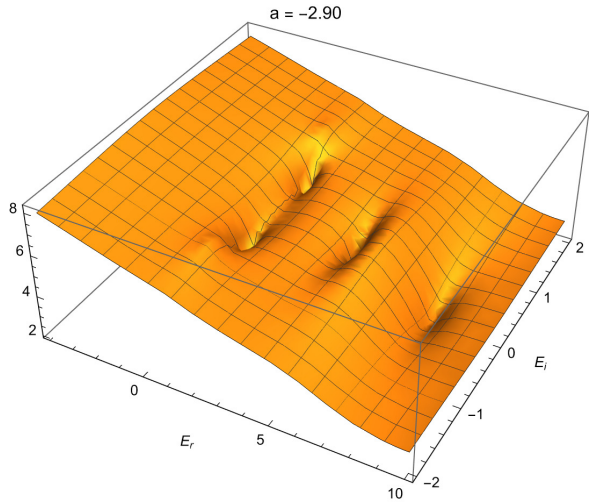

FIGURE 6. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -2.90$

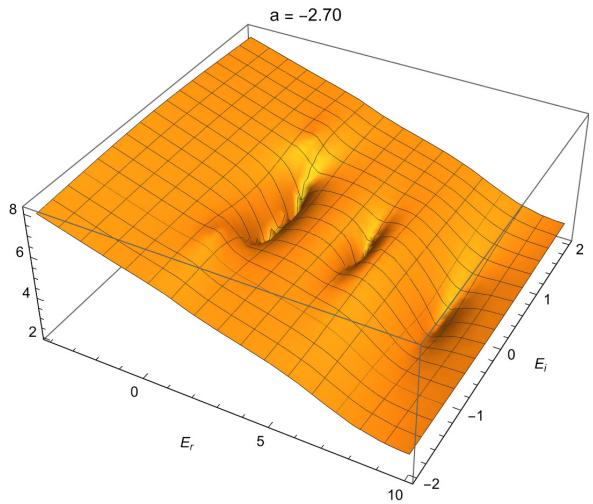

FIGURE 7. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -2.70$

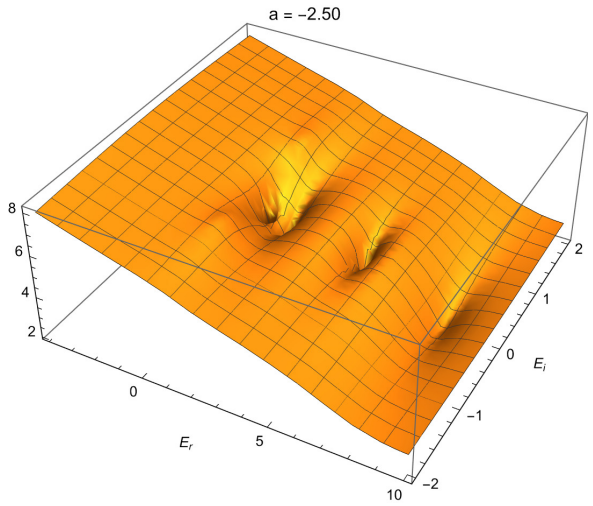

FIGURE 8. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -2.50$

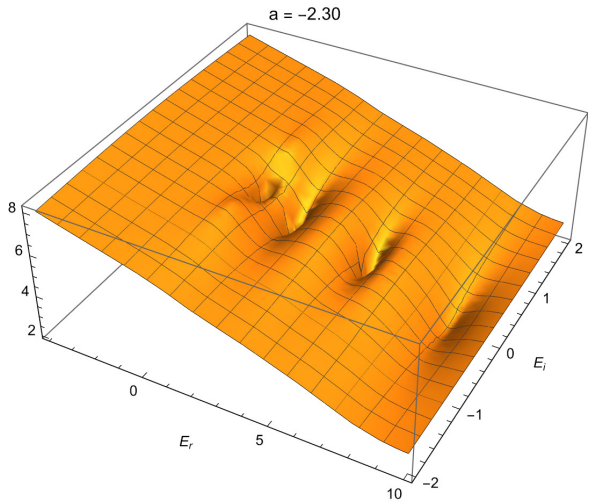

FIGURE 9. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -2.30$

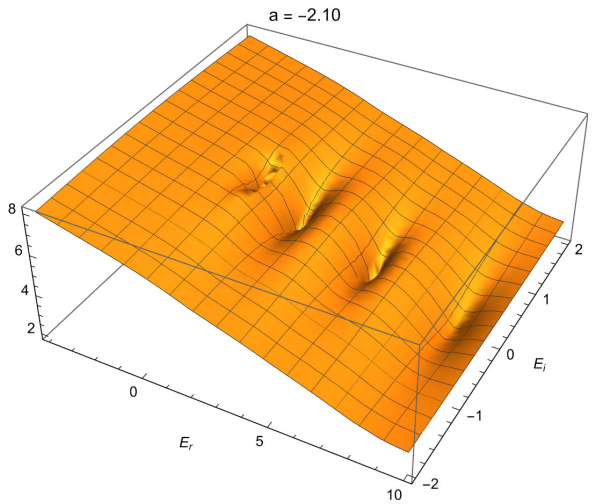

FIGURE 10. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -2.10$

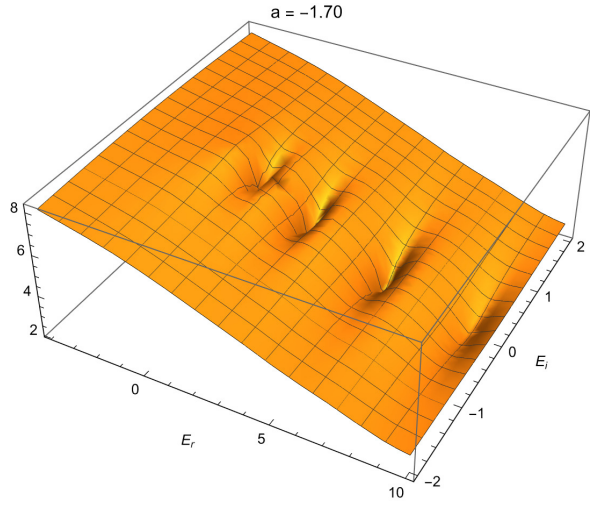

Figure 11. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = -1.70$

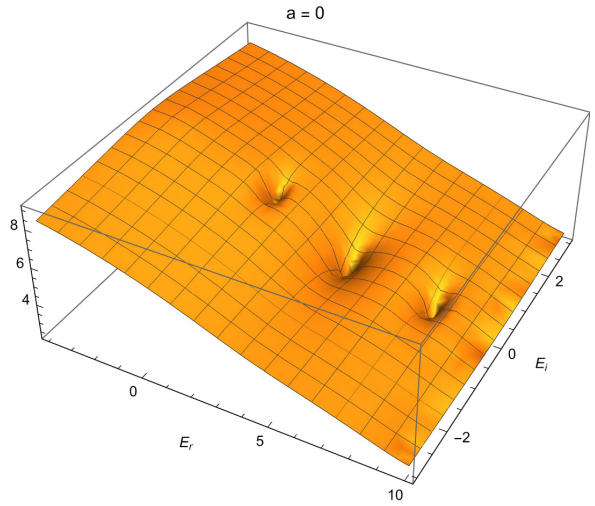

Figure 12. $Log_{10}(\lambda_{40}(E))$ for PT-breaking regime, $-3.30 \leq a \leq -1.70$ for $V(x) = ix^3 + iax$, $a = 0.00$

$-3.30, -2, 90, -2.70, -2.50, -2.30, -2.10, -1.70$ and 0. These parameter values were chosen since it is known that PT-symmetry breaking occurs at $a_{c_1} = -2.611809356$ (as well as at $a_{c_2} = -5.375879629$) [8, 25].

Figure 7 shows the behavior of the physical energies (i.e. defined by the local minima), for $a = -2.70 \approx a_{c_1}$, the critical value for the onset of symmetry breaking. For this same $a = -2.70$, Figure 4 shows the behavior of successive $\lambda_N(E)$ surfaces for $N = 20, 30, 40, 50$. Within the two dimensional graphical renderings, we see similar behaviors to that in Figures 1-3. We can implement the same OPPQ-BM bounding analysis used previously, for hermitian systems, to bound the real and imaginary parts of the *discrete state* real/complex energies. The nesting of the respecive $\lambda_N(E_r, E_i)$ in Figure 4 shows the viability of the previous OPPQ-BM analysis for bounding the real and imaginary parts of the complex-plane energies. This is the focus of a future work.

We note that for $a = 0$, the local minima in Figure 12 correspond, approximately (due to the low order, $N = 40$) to the PT-symmetric states with energies $E_0 = 1.15626707198811$, $E_2 = 4.10922875280956$, $E_3 = 7.56227385497590$ and $E_4 = 11.31442182025857$ (not shown). These were determined by EMM [8] and OPPQ-AM [10].

11. Conclusions

We have demonstrated the effectiveness of a new eigenenergy bounding procedure implementable for multidimensional discrete states regardless of the hermitian or non-hermitian character of the associated Schrödinger operator. The discussion centered on several one dimensional systems of this type. The extension to multidimensions have been given elsewhere [9]. The approach advocated here is purely algebraic.

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